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Characterization of the Bose-glass phase in low-dimensional lattices

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We study by numerical simulation a disordered Bose-Hubbard model in low-dimensional lattices. We show that a proper characterization of the phase diagram on finite disordered clusters requires the knowledge of probability distributions of physical quantities rather than their averages. This holds in particular for determining the stability region of the Bose-glass phase, the compressible but not superfluid phase that exists whenever disorder is present. This result suggests that a similar statistical analysis should be performed also to interpret experiments on cold gases trapped in disordered lattices, limited as they are to finite sizes.

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Introduction – The impressive progresses in experiments with ultra-cold gases trapped in optical lattices have revived interest in old yet fundamental issues of many-body physics. [1] In fact, these systems give the unique opportunity to experimentally realize simple many-body models, like the Bose or Fermi Hubbard models, which are believed to capture the essential physics underneath important phenomena, like for example superfluidity or the Mott metal-insulator transition.

One of the first successes of these experiments has been the observation of a superfluid to Mott insulator transition in bosonic atoms trapped in optical lattices upon varying the relative strengths of interaction and inter-well tunneling. [2] The possibility of introducing and tuning disorder, through speckles or additional incommensurate lattices, also led to the observation of Anderson localization for weakly interacting Bose gases. [3, 4] These important achievements progressively opened the way towards the challenging issue of realizing and studying a Bose-Hubbard model in the presence of disorder. Preliminary attempts to measure the excitation spectrum of interacting bosons in a disordered lattice, [5] have been performed by using Bragg spectroscopy. [6]

The phase diagram of a disordered Bose-Hubbard model is supposed to include three different phases. [7, 8] When the interaction is strong and the number of bosons is a multiple of the number of sites, the model should describe a Mott insulator, with bosons localized in the potential wells of the optical lattice. This phase is not superfluid nor compressible. When both interaction and disorder are weak, a superfluid and compressible phase must exist. These two phases are also typical of clean systems. In the presence of disorder a third phase arises: the so-called Bose glass, which is compressible but not superfluid. [8] Indeed, when disorder is very strong, bosons localize in the deepest potential wells, which are randomly distributed. The coherent tunneling of a boson

between these wells is suppressed just as in the usual Anderson localization, hence the absence of superfluidity, in spite of the fact that displacing a boson from one well to another one may cost no energy, hence a finite compressibility. Based on the same single-particle description used for explaining Anderson localization, it was argued that disorder prevents a direct superfluid to Mott insulator transition, [8] a speculation that has been subject to several theoretical studies. [9–16]

A simple way to justify the validity of the single-particle arguments is to imagine that the few carriers, which are released upon doping a Mott insulator, effectively behave as bosons at low density. In this case the single-particle Anderson localization scenario is likely to be applicable since the few interacting bosons occupy strongly localized states in the Lifshitz tails. The implicit assumption is that the Mott-Hubbard side bands survive in the presence of disorder and develop Lifshitz's tails that fill the Mott-Hubbard gap. This scenario is quite appealing hence worth to be investigated theoretically. However, a direct comparison of theory with experiments has to face the problem that experiments on cold gases are unavoidably limited to finite systems with hundreds of sites and finite number of disorder realizations. Therefore, objects like Lifshitz's tails, which arise from rare disorder configurations, might not be easily accessible. This fact demands an effort to identify salient features of the Bose glass that may distinguish the latter from a superfluid or a Mott insulator already on finite systems.

This is actually the scope of this Letter. Specifically, we are going to show that the statistical distribution of the energy gaps extracted by a numerical simulation of finite size systems is a significant property that can discriminate among different phases. The numerical simulation have been carried out for a single chain, a two- and three-leg ladder system and finally for a genuine two-

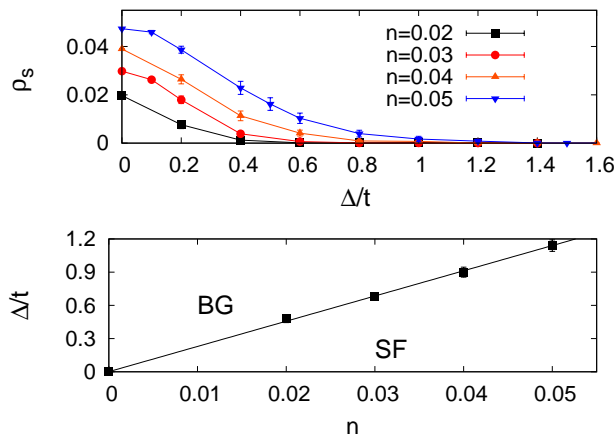


FIG. 1: (Color on-line) Upper panel: superfluid stiffness ρ_s as a function of the disorder strength Δ/t for different densities of hard-core bosons. Lower panel: low-density phase diagram of the hard-core bosonic model. Calculations have been done on a 2×50 ladder system.

dimensional lattice. The ladder systems are of interest because they can be experimentally realized, not only in optical lattices but also in magnetic materials. Indeed, very recent neutron scattering data reported the evidence of the spin-analogous of a Bose-glass phase in a spin-ladder compound in which disorder was induced by random chemical substitution. [17] Finally, we shall also discuss how the probability distribution of the energy gaps could be experimentally accessed.

Model – The simplest Hamiltonian that contains the basic ingredients of strong correlations and disorder is

$$\mathcal{H} = -\frac{t}{2} \sum_{\langle i,j \rangle} b_i^\dagger b_j + h.c. + \sum_i \left(\frac{U}{2} n_i (n_i - 1) + \epsilon_i n_i \right), \quad (1)$$

where $\langle \dots \rangle$ indicates nearest-neighbor sites, b_i^\dagger (b_i) creates (destroys) a boson on site i , and $n_i = b_i^\dagger b_i$ is the local density operator. The on-site interaction is parametrized by U , whereas the local disordered potential is described by random variables ϵ_i that are uniformly distributed in $[-\Delta, \Delta]$. Here, we consider bosons on a one-dimensional (1D) chain, N -leg ladders, and a two-dimensional (2D) square lattice, and study model of Eq. (1) by Green's function Monte Carlo with a fixed number M of bosons on L sites, $n = M/L$ being the average density. In realistic experimental setups, a two-leg ladder can be realized through a double well potential along a direction (say, x), [18] a potential creating a cigar geometry in the z -axis, and finally a periodic potential along z . [19]

Results – Before considering the case of finite U/t , let us briefly discuss the limit of hard-core bosons (i.e., $U = \infty$) at low densities. Fig. 1 shows the low-density phase diagram on a two-leg ladder. We find that for any finite disorder Δ , the low-density phase is a Bose

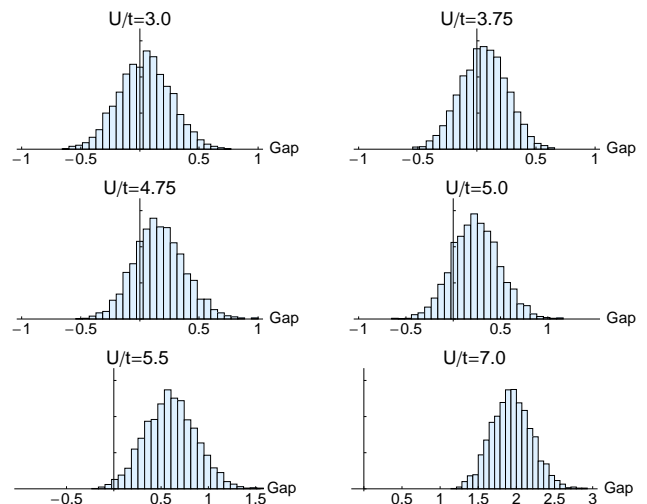


FIG. 2: Distribution $P(E_g)$ of the gap in the 1D Bose-Hubbard model for different values of U/t and $L = 60$ sites.

glass that turns superfluid above a critical density. In other words, the trivial Mott insulator with zero (or one) bosons per site is indeed separated from the superfluid phase by a Bose glass. We emphasize that the existence of a superfluid phase for hard-core bosons in a two-leg ladder is *per se* remarkable. Indeed, in a single chain with nearest-neighbor hopping, hard-core bosons are equivalent to spinless fermions, which Anderson localize for any density and in any dimension $D \leq 2$. Consequently, hard-core bosons on a single chain are never superfluid. Already in a two-leg ladder, hard-core bosons start to behave differently from spinless fermions. Indeed, while the latter ones remain always localized, the former ones show a superfluid phase. We just mention that the same occurs also on a single chain with longer-range hopping.

We now turn to finite on-site interactions and consider the case with $n = 1$. The Bose-Hubbard model has been extensively studied in recent years, [9–16] with special focus on the question whether a direct superfluid to Mott insulator transition does exist or not. This issue has been finally solved only recently. The solution is based on the observation that, if the disorder strength Δ is larger than half of the energy gap of the clean Mott insulator E_g^{clean} , then the ground state must be compressible, otherwise is incompressible. [15, 20] Therefore, the independent measurements of the superfluid stiffness ρ_s at finite Δ and of the clean Mott gap E_g^{clean} allow a precise determination of the phase boundaries between different phases and demonstrate unambiguously the existence of a Bose glass in between the superfluid and Mott phases. [15, 16] The above prescription is very effective in a numerical simulation since both ρ_s with disorder and E_g^{clean} without disorder can be determined quite accurately. On the other hand, it would be desirable to have simple instruments to establish directly the nature of the phase of a given

system in a realistic finite-size experimental setup. In a clean system, this program can be accomplished by measuring the gap, conventionally defined by $E_g = \mu^+ - \mu^-$, where $\mu^+ = E_{M+1} - E_M$ and $\mu^- = E_M - E_{M-1}$ (E_M being the ground-state energy with M particles). Experimental estimates for the gap have been so far obtained in ultra-cold atomic systems mainly in two ways: one consists in applying a gradient potential that compensates the Mott energy gap and allows tunneling between neighboring sites; [2] the other method exploits a sinusoidal modulation of the main lattice height for stimulating resonant production of excitations. [5, 6]

In disordered systems, the Mott gap can be overcome by transferring particles between two regions with almost flat disorder shifting the local chemical potential upward and downward, respectively. These regions may be far apart in space and represent rare fluctuations (Lifshitz's tail regions). Therefore, it is quite likely that the conventional definition of the gap, $\bar{E}_g = 1/\mathcal{N} \sum_{\alpha=1, \dots, \mathcal{N}} (\mu_{\alpha}^+ - \mu_{\alpha}^-)$, where α denote the disorder realizations, will miss the Lifshitz's tails for any accessible number of disorder realizations \mathcal{N} . This fact gives rise to a finite gap, even when the actual infinite system would be compressible. To circumvent such a difficulty, it is useful to imagine that a large systems is made by several subsystems, each represented by the L -site cluster under investigation, and construct the gap by using μ^+ and μ^- from *different* disorder realizations. In other words, one could define an alternative estimate of the gap as $E_g^{\min} = \min_{\alpha, \beta} |\mu_{\alpha}^+ - \mu_{\beta}^-|$, with all the disorder realizations α and β . In the limit of very large systems where boundary effects become negligible, E_g^{\min} must eventually coincide with \bar{E}_g . In finite systems the two estimates differ, nevertheless we believe that E_g^{\min} is more representative since it can capture the phenomenon underneath the Lifshitz's tails, as we are going to show numerically. Besides E_g^{\min} , one can determine the full gap distribution, $P(E_g) = \sum_{\alpha, \beta} \delta(E_g - \mu_{\alpha}^+ + \mu_{\beta}^-)$, which we will show has remarkable properties. We mention that, by our definition, $P(E_g < 0)$ could well be finite on finite systems, although it must vanish in the thermodynamic limit where $P(E_g)$ becomes peaked at a single positive (or vanishing) value, i.e., the actual gap. In experiments with ultra-cold atoms, both E_g^{\min} and $P(E_g)$ could be accessed by measuring *separately* μ^+ and μ^- for different disorder realizations. For instance, one could measure the energy releases E_M^{rel} of falling atoms when the trap is turned off with the reference number of particles M and with numbers $M \pm M'$. For $M' \ll M$, indeed $E_{M+M'}^{\text{rel}} - E_M^{\text{rel}} \simeq M' \mu^+$ and $E_M^{\text{rel}} - E_{M-M'}^{\text{rel}} \simeq M' \mu^-$.

Let us start from the 1D case, whose zero-temperature phase diagram has been worked out by Density-Matrix Renormalization Group (DMRG). [21] At finite values of Δ , the on-site interaction U turns the Bose glass into a superfluid, which remains stable up to $U = U_{c1}$, where

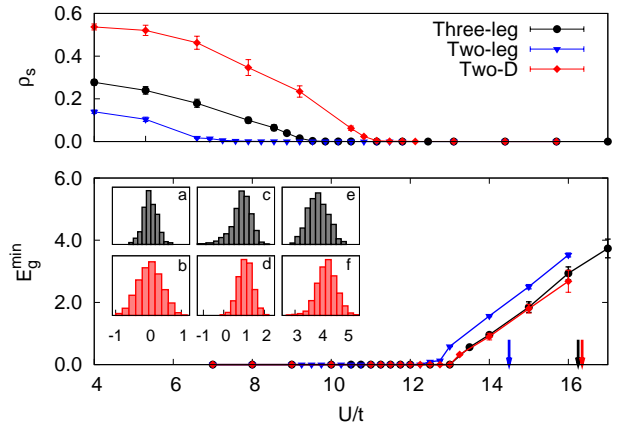


FIG. 3: (Color on-line) Upper panel: superfluid stiffness ρ_s for different clusters. Two-leg (with 2×40 sites) and three-leg (with 3×50) ladders are shown; the 2D case with a 12×12 cluster is also reported for comparison. In all cases the disorder strength is $\Delta/t = 5$. Lower panel: the same as in the upper panel for the minimum gap E_g^{\min} . Arrows indicate the opening of the charge gap according to $\Delta = E_g^{\text{clean}}/2$. The histograms for the gap are also reported for the three-leg ladders (upper row) and 2D (lower row): $U/t = 7$ (a and b), 13 (c and d), and 16 (e and f).

ρ_s vanishes. However, the system remains gapless for $U_{c1} < U < U_{c2}$, indicating the presence of a Bose-glass phase. At $U = U_{c2}$ the system turns into an incompressible Mott insulator. For $\Delta/t = 2$, we have that $U_{c1}/t \simeq 3.7$. If we use \bar{E}_g as estimator of the actual gap, we find that the Bose glass survives up to $U_{c2}/t \simeq 5$, not far from the DMRG estimate, [21] but smaller than the value predicted by the condition $\Delta = E_g^{\text{clean}}/2$, which would lead to $U_{c2}/t \simeq 6.9$. As discussed before, this discrepancy arises by the inability to catch rare disorder configurations, which could be overcome by analyzing the minimum gap E_g^{\min} and the full distribution probability $P(E_g)$. Indeed, when using E_g^{\min} as a detector of gapless excitations, we obtain an estimate of $U_{c2}/t \simeq 6.2$, much closer to the value $U_{c2}/t \simeq 6.9$. As far as $P(E_g)$ is concerned, we note that it behaves quite differently in the three different phase, see Fig. 2. As long as the phase is superfluid, $P(E_g)$ is peaked at $E_g = 0$. In the Bose glass, $P(E_g)$ is instead peaked at a finite $E_g > 0$, yet $P(0)$ stays finite. In the Mott insulator, $P(E_g)$ remains peaked at a positive E_g but $P(0) = 0$. This suggests that $P(E_g)$ could be an efficient tool for discriminating between the different phases.

Let us now analyze the evolution of the phase diagram when the 2D limit is approached by increasing the number of legs. Moving from $D = 1$ to $D = 2$, the stability region of the Bose glass is expected to shrink, [8] making its observation in experiments more and more difficult. In Fig. 3, we report our results for two- and three-leg ladders, and for comparison, also the 2D limit (evaluated

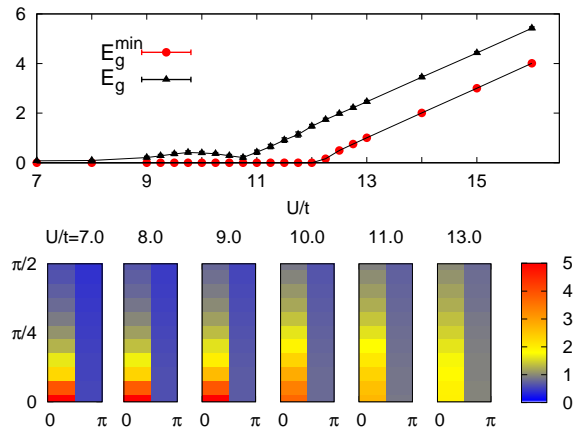


FIG. 4: (Color on-line) Upper panel: variational results for the excitation gap for a 2×40 ladder. Lower panels: momentum distribution n_k for the same cluster.

for a rather small 12×12 cluster). In this case, we take $\Delta/t = 5$, in order to have a larger Bose-glass region in between the superfluid and the Mott phases. In 1D, for such large disorder strength no superfluidity is found at all. By increasing the number of legs, we rapidly converge to the 2D results: this fact is particularly clear from the data on the gap. Both the results on the minimum gap and the ones that come from $\Delta = E_g^{\text{clean}}/2$ shows that the critical U for the Mott transition is almost the same for three legs and 2D. Also the superfluid stiffness ρ_s seems to rapidly converge from below to the 2D limit. We also find that the behavior of $P(E_g)$ is qualitatively similar to what found in 1D, confirming that it can actually discriminate among the different phases. We mention that, should we use as estimator of the gap \bar{E}_g , we would have concluded that the Bose glass never exists in 2D and that a direct superfluid to Mott insulator transition occurs. The use of E_g^{\min} instead demonstrates that the Bose glass does exist also in 2D and always intrudes between the superfluid and the Mott insulator.

We finish by showing variational results for the momentum distribution $n_k = \langle b_k^\dagger b_k \rangle$, obtained by the technique outlined in Ref. [22]. We just recall that this variational approach is based upon a Jastrow wave function and is able to describe equally well superfluid, Bose-glass, and Mott insulating states. In Fig. 4, we show the results for a 2×40 ladder and different values of U/t (we also report the results for the variational gap). Since, this is an almost 1D system, no condensation fraction is found (i.e., $n_0/L \rightarrow 0$ in the thermodynamic limit). However, the superfluid phase is characterized by quasi-long-range order with a cusp in n_k and a logarithmic divergent n_0 . On the other hand, both the Bose-glass and the Mott phases have a smooth momentum distribution, with $n_0 \rightarrow \text{const}$ in the thermodynamic limit.

Conclusions – We have presented a detailed study

of the ground-state properties of the disordered Bose-Hubbard model in low-dimensional lattices, relevant for on-going experiments with cold atomic gases trapped in optical lattices. We have determined the distribution probability of the gap on finite sizes and shown that it contains useful information. In particular, we have found that the Bose-glass is characterized by a broad distribution of the gap that is peaked at finite energy but extends down to zero, a shape remarkably reminiscent of preformed Hubbard sidebands with the Mott gap completely filled by Lifshitz’s tails. The Mott transition occurs when these tails terminate at finite energy. On the contrary, the gap distribution in the superfluid phase turns out to be strongly peaked at zero energy. These results suggest a simple and efficient way to discriminate between different phases in experiments, which, being performed on finite systems, suffer from the same size limitations as our simulations.

We have also investigated the disordered Bose-Hubbard model on N -leg ladder systems, emphasizing that these geometries could be quite useful to study the evolution from one to two spatial dimensions. Experiments with both cold atomic gases and magnetic systems are becoming now possible on ladders and our calculations represent an important benchmark in this direction.

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